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Review and analysis of biomass gasification models

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ABSTRACT

The use of biomass as a source of energy has been further enhanced in recent years and special attention has been paid to biomass gasification. Due to the increasing interest in biomass gasification, several models have been proposed in order to explain and understand this complex process, and the design, simulation, optimisation and process analysis of gasifiers have been carried out. This paper presents and analyses several gasification models based on thermodynamic equilibrium, kinetics and artificial neural networks. The thermodynamic models are found to be a useful tool for preliminary comparison and for process studies on the influence of the most important fuel and process parameters. They have the advantage of being independent of gasifier design, but they cannot give highly accurate results for all cases. The kinetic-based models are computationally more intensive but give accurate and detailed results. However, they contain parameters that limit their applicability to different plants.

Contents

1. Introduction and objectives

As we face the problems of global warming and climate change, substantial research and development has focused on the use of biomass as an alternative to fossil fuels. The widespread availability of biomass has been widely recognised, as has its potential to supply much larger amounts of useful energy with fewer environmental impacts than fossil fuels [1].

Biomass can be converted into commercial products via either biological or thermochemical processes [2–4]. Biological conversion of low-value lignocellulosic biomass still faces challenges related to low economy and efficiency [2]. Combustion, pyrolysis and gasification are the three main thermochemical conversion methods. Biomass is traditionally combusted to supply heat and power in the process industry. The net efficiency for electricity generation from biomass combustion is usually very low, ranging from 20% to 40% [3]. Biomass cofired in existing combustors is usually limited to 5–10% of the total feedstock due to concerns about plugging existing coal feed systems [4]. Pyrolysis converts biomass into bio-oil in the absence of oxygen (O_2). The limited uses and difficulty in downstream processing of bio-oil have restricted the wide application of biomass pyrolysis technology [5].

Gasification converts biomass through partial oxidation into a gaseous mixture, small quantities of char and condensable compounds. It is considered one of the most efficient ways of converting the energy embedded in biomass, and it is becoming one of the best alternatives for the reuse of waste solids.

From time to time, attempts are made to explain the complex nature of gasification. The time has come to review gasification process modelling in order to highlight the role of gasification

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models. This review aims to compare and analyse various biomass gasification models presented by different authors.

2. Biomass gasification principles and technologies

Gasification is partial thermal oxidation, which results in a high proportion of gaseous products (CO_2, water, carbon monoxide, hydrogen and gaseous hydrocarbons), small quantities of char (solid product), ash, and condensable compounds (tars and oils). Steam, air or oxygen is supplied to the reaction as an oxidising agent. The gas produced can be standardised in its quality and is easier and more versatile to use than the original biomass (e.g. it can be used to power gas engines and gas turbines or as a chemical feedstock for the production of liquid fuels). Gasification adds value to low- or negative-value feedstock by converting it into marketable fuels and products.

The chemistry of biomass gasification is quite complex. Broadly speaking, the gasification process consists of the following stages [6–9]:

- *Drying*. In this stage, the moisture content of the biomass is reduced. Typically, the moisture content of biomass ranges from 5% to 35%. Drying occurs at about 100–200 °C with a reduction in the moisture content of the biomass of <5%.
- *Devolatilisation* (*pyrolysis*). This is essentially the thermal decomposition of the biomass in the absence of oxygen or air. In this process, the volatile matter in the biomass is reduced. This results in the release of hydrocarbon gases from the biomass, due to which the biomass is reduced to solid charcoal. The hydrocarbon gases can condense at a sufficiently low temperature to generate liquid tars.
- *Oxidation*. This is a reaction between solid carbonised biomass and oxygen in the air, resulting in formation of CO_2. Hydrogen present in the biomass is also oxidised to generate water. A large amount of heat is released with the oxidation of carbon and hydrogen. If oxygen is present in substoichiometric quantities, partial oxidation of carbon may occur, resulting in the generation of carbon monoxide.
- *Reduction*. In the absence (or substoichiometric presence) of oxygen, several reduction reactions occur in the 800–1000 °C temperature range. These reactions are mostly endothermic. The main reactions in this category are as follows:

◦ Water–gas reaction:

$$C + H_2O \rightarrow CO + H_2 - 131.4\,kJ/gmol \tag{1}$$

◦ Bounded reaction:

$$C + CO_2 \leftrightarrow 2CO - 172.6\,kJ/gmol \tag{2}$$

◦ Shift reaction:

$$CO_2 + H_2 \leftrightarrow CO + H_2O - 42\,kJ/gmol \tag{3}$$

◦ Methane reaction:

$$C + 2H_2 \leftrightarrow CH_4 + 75\,kJ/gmol \tag{4}$$

Gasification reactor designs have been researched for more than a century, which has resulted in the availability of several designs at the small and large scales. They can be classified in several ways [10]:

- *By gasification agent*: Air-blown gasifiers, oxygen gasifiers and steam gasifiers.
- *By heat source*: Auto-thermal or direct gasifiers (heat is provided by partial combustion of biomass) and allothermal or indirect gasifiers (heat is supplied by an external source via a heat exchanger or an indirect process).
- *By gasifier pressure*: Atmospheric or pressurised.
- *By reactor design*:
  - Fixed-bed (updraft, downdraft, cross-draft and open-core): The fixed-bed gasifier has a bed of solid fuel particles through which the gasifying media and gas either move up (updraft), move down (downdraft) or are introduced from one side of the reactor and are released from the other side on the same horizontal level (cross-draft). It is the simplest type of gasifier, usually consisting of a cylindrical space for fuel and gasifying media with a fuel-feeding unit, an ash-removal unit and a gas exit. In the fixed-bed gasifier, the fuel bed moves slowly down the reactor as the gasification occurs. Fixed-bed gasifiers are simple to construct and generally operate with high carbon conversion, long solid residence time, low gas velocity and low ash carry-over [11,12].
  - Fluidised-bed (bubbling, circulating and twin-bed): The gasifying agent is blown through a bed of solid particles at a sufficient velocity to keep the particles in a state of suspension. Fuel particles are introduced at the bottom of the reactor, are very quickly mixed with the bed material, and almost instantaneously are heated up to the bed temperature. As a result of this treatment, the fuel is pyrolysed very fast, resulting in a component mix with a relatively large amount of gaseous materials. Further gasification and tar-conversion reactions occur in the gas phase. Twin-bed gasification uses two fluidised-bed reactors. The biomass enters the first reactor, where it is gasified with steam, and the remaining char is transported to the second reactor, where it is burnt with air to produce heat. The heat is transported to the gasification reactor by the bed material, normally sand. The flue gas and the product gas have two separate exits.
  - Entrained-flow: These gasifiers are commonly used for coal because they can be slurry-fed in direct gasification mode, which makes solid fuel feeding at high pressures inexpensive. These gasifiers are characterised by short residence time, high temperatures, high pressures and large capacities [13].
  - Stage gasification with physical separation of pyrolysis, oxidation and/or reduction zones.

Table 1 compares various types of biomass gasifiers.

A review of gasifier manufacturers in Europe, the United States and Canada [14] identified 50 manufacturers offering commercial gasification plants, of which 75% were of the fixed-bed downdraft type, 20% were fluidised-bed systems, 2.5% were of the updraft type, and 2.5% were of various other designs.

3. Performance of biomass gasifiers

The performance of biomass gasifiers could be characterised by several parameters. Here, we will review two such parameters: producer-gas composition, which directly influences the heating value of the gas, and gasification efficiency.

The composition of the gas obtained from a gasifier depends on a number of parameters, such as fuel composition, gasifying medium, operating pressure, temperature, moisture content of the fuels, mode of bringing the reactants into contact inside the gasifier (gasifier design), etc., and this is why it is very difficult to predict the exact composition of the gas from a gasifier [15]. By way of example, Table 2 shows typical gas composition data as obtained from commercial wood downdraft gasifiers operated on low- to medium-moisture-content fuels [16] and Table 3 shows typical producer-gas composition and operating conditions for atmospheric bubbling fluidised-bed gasifiers [17].

The oxidant or gasifying agents can be air, pure O_2, steam, CO_2 or mixtures thereof. Air, while a cheap and widely used gasifying agent, contains a large amount of nitrogen, which lowers the

Table 1
Salient features and comparative evaluation of different designs of biomass gasifiers [9,106,107].

Downdraft	Updraft
Simple and proven technology.	Simple and proven technology.
Fuel specificity in terms of both type and size.	Low exit gas temperature.
Suitable for biomasses with low moisture.	High thermal efficiency.
Producer gas with moderate calorific value and low tar and ash (or particulate) content.	Producer gas with moderate calorific value but high tar and ash (or particulate) content.
High exit gas temperature.	High residence time of solids.
Suitable for capacities of 20–200 kW.	High overall carbon conversion.
High residence time of solids.	Extensive gas cleanup required before it can be used in engines.
High overall carbon conversion.	Suitable for capacities up to 250 kW.
Limited scale-up potential with maximum capacity of 250 kW.	Limited scale-up potential.
Bubbling fluidised bed	Circulating fluidised bed
High fuel flexibility in terms of both size and type.	High fuel flexibility in terms of both size and type.
Flexibility of operation at loads lower than design load.	Flexibility of operation at loads lower than design load.
Ease of operation.	Ease of operation.
Low feedstock inventory.	Low feedstock inventory.
Good temperature control and high reaction rates.	Good temperature control and high reaction rates.
Good gas–solid contact and mixing.	In-bed catalytic processing possible.
In-bed catalytic processing possible.	Producer gas with moderate tar levels but high particulates.
Producer gas with moderate HHV but low tar levels and high particulates.	High carbon conversion.
Carbon loss with ash.	Good gas–solid contact and mixing.
High conversion efficiency.	Suitable for large-scale capacities (up to 1 MW or even higher).
Suitable for large-scale capacities (up to 1 MW or even higher).	High conversion efficiency.
Good scale-up potential.	Very good scale-up potential.
Entrained-flow bed	Twin fluidised bed
Relatively complex construction and operation.	Relatively complex construction and operation.
Fuel specificity in terms of particle size (costly feed preparation).	Producer gas with moderate HHV and moderate tar levels.
Low feedstock inventory.	Cleaning of gas required before it can be fired into engines.
High temperature gives good gas quality.	In-bed catalytic conversions possible.
Problems with construction materials at high temperature.	Good gas–solid contact and mixing.
Good gas–solid contact and mixing.	Relatively low efficiency.
Producer gas with moderate HHV and low tar content.	Suitable for high specific capacities (>1 MW).
High conversion efficiency.	Good scale-up potential but relatively complex design.
Suitable for high capacities (>1 MW).	
Very good scale-up potential.	

Table 2
Typical producer-gas composition from commercial wood for downdraft gasifiers operated on low- to medium-moisture-content fuels [16].

Component	[%]
H_2	12–20
CO_2	9–15
CH_4	2–3
CO	17–22
N_2	50–54
Heating value	5–5.9 MJ/m^3

Table 3
Typical producer-gas composition and operating conditions for atmospheric bubbling fluidised-bed gasifiers [17].

	Air [108]	Steam (pure) [109]	Steam–O_2 mixtures [110]
Operating conditions			
ER	0.18–0.45	0	0.24–0.51
S/B (kg/kg daf)	0.08–0.66	0.53–1.10	0.48–1.11
T (°C)	780–830	750–780	785–830
Gas composition			
H_2 (vol%, dry basis)	5.0–16.3	38–56	13.8–31.7
CO (vol%, dry basis)	9.9–22.4	17–32	42.5–52.0
CO_2 (vol%, dry basis)	9.0–19.4	13–17	14.4–36.3
CH_4 (vol%, dry basis)	2.2–6.2	7–12	6.0–7.5
C_2H_n (vol%, dry basis)	0.2–3.3	2.1–2.3	2.5–3.6
N_2 (vol%, dry basis)	41.6–61.6	0	0
Steam (vol%, wet basis)	11–34	52–60	38–61
Yields			
Tars (g/kg daf)	3.7–61.9	60–95	2.2–46
Char (g/kg daf)	na	95–110	5–20
Gas (Nm^3/kg daf)	1.25–2.45	1.3–1.6	0.86–1.14
LHV (MJ/Nm^3)	3.7–8.4	12.2–13.8	10.3–13.5

na: not available; daf: dry ash-free basis; ER: equivalence ratio; S/B: steam-to-biomass ratio (H_2O (kg/h)/biomass (kg daf/h)).

heating value of the syngas produced. If pure O_2 is used as the gasifying agent, the heating value of syngas will increase but the operating costs will also increase due to the O_2 production costs. Partial combustion of biomass with air or O_2 can provide heat for drying the biomass, raising the biomass temperature and driving the endothermic gasification reactions, and generate water and CO_2 for further reduction reactions [15]. The heating value and H_2 content of the syngas can be increased if steam is used as the gasifying agent, in which case the heating value of the product gas is about 10–15 MJ/Nm^3 [17,18], compared with 3–6 MJ/Nm^3 for air gasification of biomass [19,20]. The use of CO_2 as the gasifying agent is promising because of its presence in the syngas. CO_2 with a catalyst such as Ni/Al can transform char, tar and CH_4 into H_2 and/or CO, thus increasing H_2 and CO contents [21–23]. Pure steam or CO_2 requires an indirect or external heat supply for endothermic gasification reactions [24–27]. Alternatively, a mixture of steam or CO_2 and air or O_2 can be used as the gasifying agent, and the partial combustion of biomass with air/O_2 provides the heat required for gasification [17,28–30].

Some authors, like Prins et al. [31,32], Ptasinski et al. [33] and Ptasinski [34], have focused their studies on the efficiency of biomass gasification. Efficiency is either based on energy (lower heating value, LHV) (Eq. (5)) or exergy (chemical, and chemical and physical, exergy) (Eq. (6)). All efficiencies are defined as the ratio between the exergy (energy, respectively) of the syngas to the exergy (energy, respectively) of the biomass:

$$\text{Energy efficiency}\,(\%)(\text{per kg of biomass}):\ \eta = \frac{n_{gas}\cdot \mathrm{LHV}_{gas}}{\mathrm{LHV}_{biomass}} \quad (5)$$

$$\text{Exergy efficiency}(\%)(\text{for an adiabatic gasifier using air as the gasifying medium}):\ \psi = \frac{n_{gas}\cdot(e_{ch,gas}+e_{ph,gas})}{e_{ch,biomass}+n_{air}\cdot e_{air}} \quad (6)$$

where n_{gas} is the molar amount of product gas (kmol); n_{air} is the molar amount of air (kmol); $e_{ch,gas}$ is the chemical exergy of product gas (kJ/kmol); $e_{ph,gas}$ is the physical exergy of product gas (kJ/kmol); $e_{ch,biomass}$ is the chemical exergy of biomass (kJ/kmol); e_{air} is the specific molar exergy of air (kJ/kmol).

Ptasinski [34] analysed the efficiency of biomass gasification using the triangular C–H–O diagram, considering a biomass fuel that can be represented by a general formula of $CH_{1.4}O_{0.59}N_{0.0017}$. At the equivalence ratio of 0.26, the chemical and total exergy of the gas reach the maximum at the carbon boundary. The carbon boundary point (CBP) is the optimum point for operating an air-blown gasifier and it is obtained when exactly enough gasifying medium is added to avoid carbon formation and achieve complete gasification. Desrosiers [35] and Double and Bridgwater [36] proved that the CBP is the optimum point for gasification with respect to energy-based efficiency, and Prins et al. [37] proved that it is the optimum point with respect to exergy-based efficiency, as cited by Ptasinski et al. [33]. At this point, according to Ptasinski [34], the exergetic efficiency of biomass gasification is the highest, equal to 80.5%. For gasification with steam, operation at the CBP is also optimal from the point of view of exergetic efficiency. The optimal gasification occurs at the steam-to-biomass ratio of 1.30 kg/kg and results in an overall exergetic efficiency of 87.6%. Steam gasification is thus more efficient than air gasification, but this advantage is reduced when the exergy losses during steam production are taken into account. The exergetic efficiency of gasification also depends on the chemical composition of the biofuel used as feedstock. According to Ptasinski [34], the energetic efficiencies of vegetable oil, straw, treated wood, untreated wood and grass are comparable with that of coal, whereas the efficiencies of sludge and manure are considerably lower (Fig. 1). This can be expected, because gasification at the optimum operating point is not possible for these streams. In sludge and manure gasification, oxygen is added mainly to generate heat and to evaporate moisture present in the fuel. If the exothermic oxidation reactions could drive endothermic gasification reactions, rather than the endothermic evaporation of water, the gasifier would work much more efficiently. Efficiency based on chemical exergy is higher for coal and vegetable oil than for the other biomass streams. The same trends can be observed for gasification efficiencies based on chemical and physical exergy. Because coal and vegetable oil are gasified at higher temperatures, their gasification efficiencies are relatively much improved by the inclusion of the physical exergy. Drier biomass, such as treated wood or straw, may be slightly preferred over fresh biomass, such as untreated wood and grass. These results assume that gasification reaction rates are fast enough and residence time is long enough for the equilibrium state to be reached.

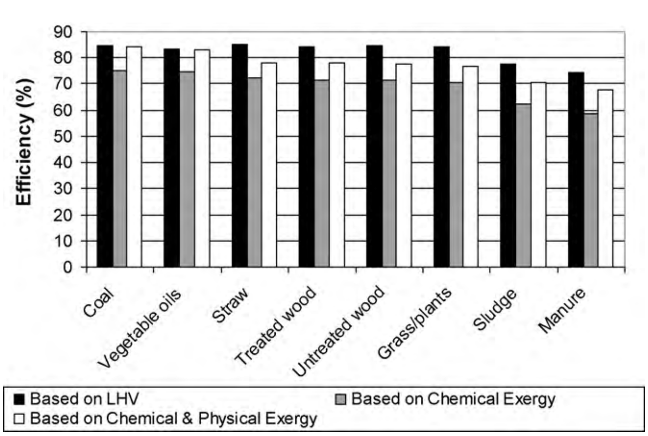


Fig. 1. Comparison of gasification efficiency of various fuels [34].

4. Biomass gasification models

The efficient operation of a biomass gasifier depends on a number of complex chemical reactions, including fast pyrolysis, partial oxidation of pyrolysis products, gasification of the resulting char, conversion of tar and lower hydrocarbons, and the water–gas shift reaction. These complicated processes, coupled with the sensitivity of the product distribution to the rate of heating and residence time in the reactor, required the development of mathematical models. The main goals of these models are to study the thermochemical processes during the gasification of the biomass and to evaluate the influence of the main input variables, such as moisture content, air/fuel ratio, producer-gas composition and the calorific value of the producer gas.

Some studies only consider the final composition of chemical equilibrium, while others take into account the different processes along the gasifier, distinguishing at least two zones. The models can be divided into kinetic rate models, thermodynamic equilibrium models and neural network models. Some models use the process simulator Aspen Plus [101] combining thermodynamic and kinetic rate models.

4.1. Kinetic rate models

Kinetic models provide essential information on kinetic mechanisms to describe the conversion during biomass gasification, which is crucial in designing, evaluating and improving gasifiers. These rate models are accurate and detailed but are computationally intensive [38]. Nevertheless, numerous researchers have focused extensively on kinetic models of biomass gasification: Wang and Kinoshita [39], Di Blassi [102], Fiaschi and Michelini [40], Giltrap et al. [41], Yang et al. [42], Roshmi et al. [43], Dennis et al. [44], Babu and Sheth [54], Radmanesh et al. [45], Gobel et al. [46], Sharma [38], Fermoso et al. [47], Zhong et al. [48] and Roy et al. [49].

Kinetic models describe the char reduction process using kinetic rate expressions obtained from experiments and permit better simulation of the experimental data where the residence time of gas and biomass is relatively short.

The kinetic model proposed by Wang and Kinoshita [39] is based on a mechanism of surface reactions in the reduction zone assuming a given residence time and reaction temperature. Giltrap et al. [41] developed a model of the reduction zone of a downdraft biomass gasifier to predict the composition of the producer gas under steady-state operation, adopting the kinetic rate expressions of Wang and Kinoshita [39]. The accuracy of the model is limited by the availability of data on the initial conditions at the top of the reduction zone; pyrolysis and cracking reactions are not considered because the number of possible pyrolysis products, along with all the possible reactions and intermediate products, would make the model very complex. It assumes that all the oxygen from the air inlet is combusted to CO_2 and that the pyrolysis products are completely cracked. Solid carbon, in the form of char, is considered to be present throughout the reduction region. It is assumed that the char reactivity factor (CRF), which represents the reactivity of the char and is a key variable in the simulation, is taken as constant throughout the reduction zone. These authors tested the model with experimental data for two different downdraft gasifiers (Chee [50,105]). Fig. 2 compares the composition of the dry producer gas predicted by this model with those found experimentally. The model produced reasonable agreement with the experimental results for all components except CH_4. According to Giltrap et al. [41], this over-prediction was the result of the assumption that O_2 in the air reacts only with char. The pyrolysis products are cracked in a region of high temperature and in the presence of O_2, so it is probable that some of the CH_4 produced will undergo combustion

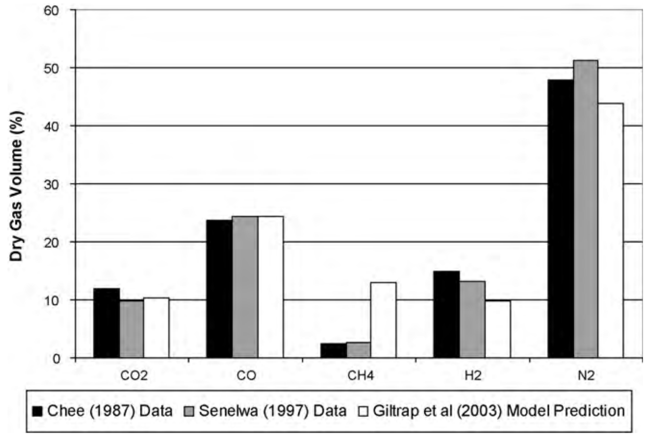


Fig. 2. Predicted results from the model of Giltrap et al. [41] compared with experimental data from Chee [105] and Senelwa [50].

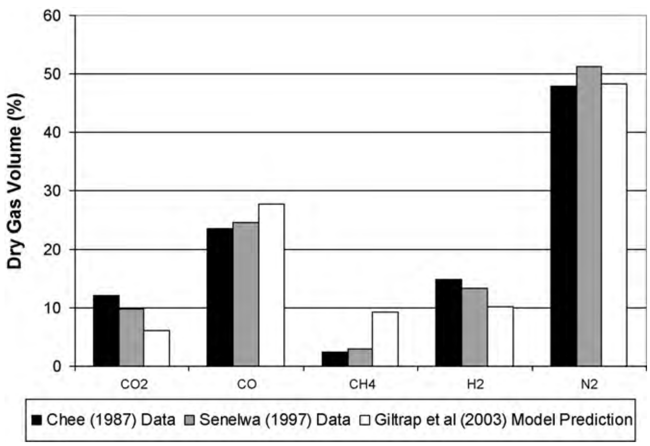


Fig. 3. Predicted results from the model of Giltrap et al. [41] compared with experimental data from Chee [105] and Senelwa [50] when the initial conditions of the model assumed that the CH_4 produced by the cracking of pyrolysis products reacts with O_2 entering the gasifier through the air inlet.

with O_2. Fig. 3 shows the results when the initial gas concentration is altered under the assumption that all of the O_2 in the air reacts with the CH_4 from the cracking of the pyrolysis gas. This assumption reduces the amount of CH_4 predicted, but the prediction is still higher than the concentrations found experimentally.

Jayah et al. [51] developed a model based in the early work of Chen [52] but with a few modifications. Chen's model was intended to estimate the length of the gasification zone and the diameter of the reactor, and to investigate the dependence of the reactor's performance on operating parameters such as feedstock moisture content, chip size, reactor insulation, input air temperature and gasifier load. Chen's model consists of three parts. The first part determines the amount of oxygen needed for a fixed input of fuel at a specific operating condition. The fuel-to-air ratio estimated from this first part of the model is then used as an input in the second part, where the drying, pyrolysis and combustion zones are all lumped together and considered as a single zone. The outputs from this "lumped" zone are the product concentrations and the temperatures of the gaseous and solid phases leaving the zone. These calculated concentrations and temperatures are then used as inputs in the third part of the model, which predicts the temperature profile along the axis of the gasification zone, the gas composition, the conversion efficiency and the length of the gasification zone at any given time interval. The main weakness of Chen's model is the over-prediction of the gas exit temperature from the "lumped" zone due to an unrealistically low estimate of heat loss and the omission of CO and H_2 in the pyrolysis gas. Jayah et al. [51] therefore introduced modifications to overcome these deficiencies and also to suit a reactor with a variable rather than constant gasification zone diameter. For this reason, the authors incorporated Milligan's [53] flaming pyrolysis sub-model instead of the algorithms used by Chen [52]. The aim of Milligan's Daming pyrolysis zone model is to calculate the composition of the product gas entering the gasification zone in terms of CO, H_2, CO_2, H_2O, CH_4 and N_2. As a result, the model used in the study by Jayah et al. [51] consists of two sub-models, namely of the Daming pyrolysis and the gasification zones. The Daming pyrolysis zone sub-model is used to determine the maximum temperature and the product concentration of the gas leaving that zone. The gasification zone sub-model assumes that a single char particle moves vertically downwards along the vertical axis of the gasifier. This sub-model includes a description of the physical and chemical processes, the flow equations, the transport phenomena and the conservation principles. The model is limited to considering the effect of packed char particles in the reduction zone.

Babu and Sheth [54] modified Giltrap's model suggesting an exponentially varying CRF in order to predict better simulation of the temperature profile in the reduction reaction zone. The CRF value was increased both linearly and exponentially along the length of the reduction bed in the model. The model was simulated with a finite difference method to predict the temperature and composition profiles in the reduction zone. The model predictions were compared with the experimental data reported by Jayah et al. [51] (Fig. 4). Simulations were performed for varying CRFs ranging from 1 to 10,000, and linearly and exponentially as well. Simulations were also performed for different values of CRF (1, 10, 100 and 1000) held constant throughout the reduction zone. The authors of the study concluded that the CRF must be varied along the reduction zone of the downdraft gasifier and that their simulated results were in very good agreement with the experimental data of Jayah et al. [51]—better, in fact, than the mathematical model of Jayah et al. [51], which considered an exponentially varying CRF value.

Recently, Sharma [38] presented a model for a downdraft gasifier in which the reduction zone was modelled using a finite rate of reaction following the chemical kinetics. The pyro-oxidation zone, prior to the reduction zone, was also modelled considering thermodynamic equilibrium. However, the author did not take into account any char combustion in the pyro-oxidation zone and also neglected the formation of methane there. The

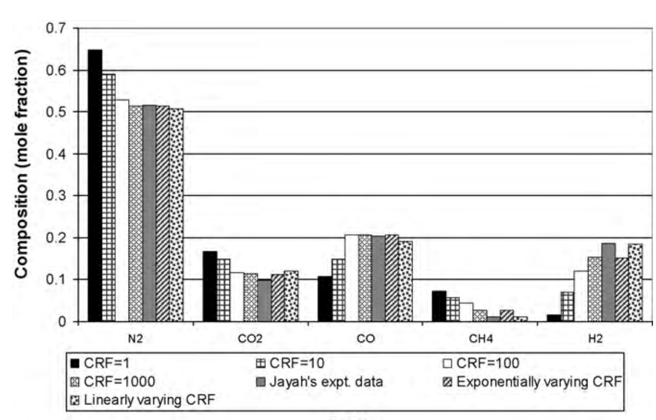


Fig. 4. Comparison of various producer-gas compositions that have varying CRF values (Babu and Seth [54]) with experimental data from Jayah et al. [51].

water–gas shift equilibrium was considered at the outlet of the pyro-oxidation zone. In the reduction zone, a linear variation of CRF was adopted. Following this previous work, Roy et al. [49] developed a model for a downdraft gasifier based on chemical equilibrium in the pyro-oxidation zone and finite-rate kinetic-controlled chemical reactions in the reduction zone. The CRF was optimised by comparing the model's predictions against the experimental results from the literature.

4.2. Thermodynamic equilibrium models

Kinetic rate models always contain parameters that limit their applicability to different plants. Thus, thermodynamic equilibrium calculations, which are independent of gasifier design, may be more suitable for process studies on the influence of the most important fuel process parameters. At chemical equilibrium, a reacting system is at its most stable composition, a condition achieved when the entropy of the system is maximised while its Gibbs free energy is minimised. However, thermodynamic equilibrium may not be achieved, mainly due to the relatively low operation temperatures (product gas outlet temperatures range from 750 to 1000 °C) (Bridgwater [106]). Nevertheless, models based on thermodynamic equilibrium have been used widely. Some recent efforts include the work done by Bacon et al. [55], Double et al. [56], Ruggiero and Manfrida [57], Zainal et al. [58], Schuster et al. [59], Altafini et al. [60], Li et al. [61,62], Melgar et al. [63], Jarungthammachote and Dutta [71,73], Yoshida et al. [64], Karamarkovic and Karamarkovic [65], Huang and Ramaswamy [66] and Haryanto et al. [67] to predict the performance of commercial gasifiers. These authors have shown reasonable agreement between equilibrium predictions and experimental data.

Equilibrium models have two general approaches: stoichiometric and non-stoichiometric. The stoichiometric approach requires a clearly defined reaction mechanism that incorporates all chemical reactions and species involved. In the non-stoichiometric approach, no particular reaction mechanisms or species are involved in the numerical simulation. The only input needed to specify the feed is its elemental composition, which can be readily obtained from ultimate analysis data [62]. The non-stoichiometric equilibrium model [68] is based on minimising Gibbs free energy in the system without specifying the possible reactions taking place. The stoichiometric chemical equilibrium model is based on selecting those species that are present in the largest amounts, i.e. those which have the lowest value of free energy of formation. As noted by Prins et al. [37], Desrosiers [35] showed that under gasification conditions (with temperatures between 600 and 1500 K) the only species present at concentrations higher than 10^{-4} mol% are CO, CO_2, CH_4, H_2, N_2, H_2O and solid carbon (graphite). For this system of species, there are three independent chemical reactions (Eqs. (1), (2) and (4)), according to Duhem's theory [69]. For the homogeneous system that consists of CO, CO_2, CH_4, H_2, N_2 and H_2O, there are two independent chemical reactions, resulting from the combination of Eqs. (1) and (2) and also Eqs. (1) and (4).

As shown by various authors [70,71], the two approaches (stoichiometric and non-stoichiometric) are essentially equivalent. A stoichiometric model may also use free energy data to determine the equilibrium constants of a proposed set of reactions.

Equilibrium models are based on some general assumptions that are in better agreement with some specific types of reactors for which equilibrium models have better predictive capabilities. Prins et al. [31] presented these assumptions:

- The reactor is implicitly considered to be zero-dimensional.
- The gasifier is often regarded as a perfectly insulated apparatus, i.e. heat losses are neglected. In practice, gasifiers have heat losses to the environment, but this term can be incorporated in the enthalpy balance of the equilibrium model.
- Perfect mixing and uniform temperature are assumed for the gasifier although different hydrodynamics are observed in practice, depending on the design of the gasifier.
- The model assumes that gasification reaction rates are fast enough and residence time is long enough to reach the equilibrium state.
- No information about reaction pathways and the formation of intermediates is given in the model.
- Tars are not modelled.

Due to these assumptions, equilibrium models yield great disagreements under some circumstances. Typical pitfalls at relatively low gasification temperatures are the overestimation of H_2 and CO yields and the underestimation of CO_2, methane, tars and char (in fact, null values for these last three components above 800 °C) [72]. For this reason, and as detailed below, several authors have modified and corrected the equilibrium model or used the quasi-equilibrium temperature (QET) approach.

Zainal et al. [58] modelled the biomass gasification process on the basis of stoichiometric thermodynamic equilibrium. They predicted the composition of the producer gas for different biomass materials. Jarungthammachote and Dutta [71] developed the thermodynamic equilibrium model based on the equilibrium constant for predicting the composition of a producer gas in a downdraft gasifier. They used coefficients for correcting the equilibrium constant of the water–gas shift reaction and the methane reaction in order to improve the model. Those coefficients were obtained from the comparison between the model and the results of other researchers' experiments. The predicted results from the modified model satisfactorily agree with experimental results reported by Jayah et al. [51] (Table 4).

Jarungthammachote and Dutta [73] applied the non-stoichiometric equilibrium model to three types of gasifiers: a central jet spouted bed, a circular split spouted bed and a spout-fluid bed. The simulation results from the model showed a significant deviation from the experimental data, especially for CO and CO_2. One important factor was carbon conversion. Thus, the model was modified to consider the effect of carbon conversion. The results improved and were closer to the experimental data (Table 5). However, this model could not give results with high accuracy for the spouted-bed gasification process. The heating value was also an important parameter because it is usually used to estimate the energy that could be gained from using that producer gas. The modified model predicted heating values that were generally higher than those from experiments because of the over-prediction of the CO content in the producer gas.

An equilibrium model for studying biomass gasification with steam in a fluidised-bed gasifier was presented by Schuster et al. [59]. The results of the equilibrium model for the gasifier (LHV × gas yield) were in the range of the measured results, though the CH_4 content in the product gas was overestimated. It

Table 4
Comparison of the results from the modified model of Jarunthammachote and Dutta [71] with the experimental data of Jayah et al. [51].

Gas composition % mol dry basis	Model data [71]		Experimental data [51]	
	MC (16%)	MC (14%)	MC (16%)	MC (14%)
H_2	16.81	16.80	17.00	12.50
CO	17.86	18.52	18.40	18.90
CH_4	1.05	1.06	1.30	1.20
CO_2	12.10	11.68	10.60	8.50
N_2	52.18	51.94	52.70	59.10
m	0.4472	0.4415	0.3361	0.3927

Table 5
Comparison between experimental results, original model and modified model of Jarunthammachote and Dutta [73].

	H_2 (vol%)	CO_2 (vol%)	CO (vol%)	CH_4 (vol%)	N_2 (vol%)	O_2 (vol%)	HHV (MJ/Nm^3)	RMS error
Central jet spouted bed at 1323.3 K								
Experiment	12.56	14.56	14.97	0.7	54.96	2.27	3.906	
Original model	11.08	2.6	30.36	∼0	55.96	–	5.44	8.020
Modified model	13.55	8.73	19.18	∼0	58.53	–	4.302	3.319
Circular split spouted bed at 1388.3 K								
Experiment	10.98	13.7	16.41	0.88	57.47	0.55	3.961	
Original model	10.26	3.17	29.23	∼0	57.34	–	5.183	6.807
Modified model	12.45	9.16	18.15	∼0	60.22	–	4.022	2.385
Spout-fluid bed ER = 0.35 at 1148.7 K								
Experiment	8.43	14.95	11.61	2.52	61.55	–	3.891	
Original model	14.99	10.42	20.68	∼0	53.9	–	4.688	5.935
Modified model	16.07	14.42	13.71	∼0	55.8	–	3.917	4.133
Spout-fluid bed ER = 0.30 at 1127.65 K								
Experiment	11.86	14.48	13.03	2.95	56.87	–	4.01	
Original model	15.45	10.43	21.08	∼0	53.3	–	4.801	4.400
Modified model	16.72	14.5	13.76	∼0	55.02	–	4.01	2.459

was shown that the discrepancies in the prediction of the gas composition did not significantly influence the overall efficiency.

Li et al. [61] used a non-stoichiometric equilibrium model (minimisation of Gibbs free energy) to predict the producer-gas composition from a circulating fluidised-bed coal gasifier. Li et al. [62] employed the equilibrium model to predict the producer-gas compositions, product heating value and cold gas efficiency for circulating fluidised-bed gasification. They observed that real gasification processes deviate from chemical equilibrium. Therefore, in order to correct the deviations, they developed a phenomenological model to modify the equilibrium-based framework to account for key non-equilibrium factors. As they knew from a pilot-plant study the experimental carbon conversion and methane yield, it was possible to correct non-equilibrium effects by withdrawing the corresponding carbon and hydrogen from the equilibrium system. Fig. 5 compares the experimental data and the predicted values from the modified model. This method was also applied successfully to coal gasification [61] and to steam–methane reforming [74], where hydrogen was preferentially removed through perm-selective membranes.

Another approach is the use QET, whereby the equilibria of the reactions defined in the model are evaluated at a temperature that is lower than the actual process temperature. This approach was introduced by Gumz [75]. For fluidised-bed gasifiers, the average bed temperature can be used as the process temperature, whereas for downdraft gasifiers, the outlet temperature at the throat exit should be used. Li et al. [61] found that the kinetic carbon conversion for pressurised gasification of sub-bituminous coal in the temperature range 747–877 °C is seen to be comparable to equilibrium predictions for a temperature about 250 °C lower. Bacon et al. [76] defined QETs for each independent chemical reaction. Based on 75 operational data points measured in circulating fluidised-bed (CFB) gasifiers operated on biomass, Kersten et al. [77] showed that, for operating temperatures in the range 740–910 °C, the reaction equilibrium of Eqs. (1), (2) and (4) should be evaluated at much lower temperatures (respectively, 531 ± 25 °C, 583 ± 25 °C and 457 ± 29 °C). These QETs appear to be independent of process temperature in this range.

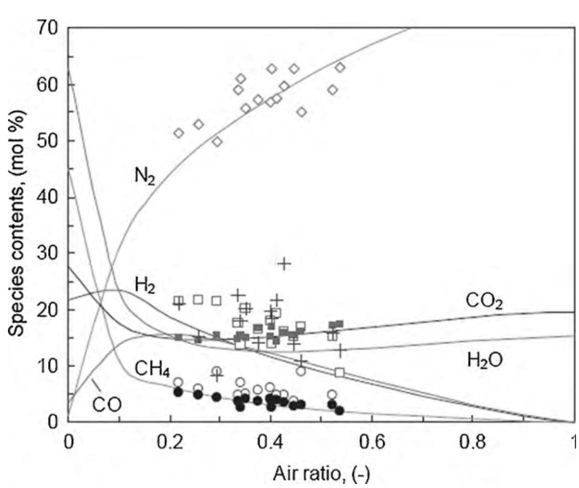


Fig. 5. Comparison between the experimental gas composition and the gas composition predicted with the modified model. Data from the study of Li et al. [62].

This literature review has shown that equilibrium models are useful tools for preliminary comparison, but that they cannot give highly accurate results for all cases. As mentioned above, thermodynamic equilibrium models do not require any knowledge of the mechanisms of transformation. Moreover, they are independent of the reactor and not limited to a specified range of operating conditions. They are valuable because they predict the thermodynamic limits of the gasification reaction system. Thus, in order to describe the behaviour of gasifiers more accurately, modifications have been made to equilibrium models. According to Villanueva et al. [72], chemical equilibrium is a good approach when simulating entrained-flow gasifiers in chemical process simulators. Similar conclusions were made, by the same authors, for downdraft fixed-bed gasifiers as long as high temperature and gas residence time are achieved in the throat. In contrast, updraft fixed-bed, dual fluidised-bed and stand-alone fluidised-bed gasifiers should be modelled by revised equilibrium models or, in some extreme cases, by detailed rate-flow models. In these gasifiers, knowledge of biomass devolatilisation is crucial for a successful prediction of performance. In dual fluidised-bed gasifiers, char is converted in the combustor, while in fluidised-bed gasifiers, char conversion is rather limited and its prediction seems to be a key parameter for proper prediction.

4.3. Aspen Plus gasification models

Some authors, trying to avoid complex processes and develop the simplest possible model that incorporates the principal gasification reactions and the gross physical characteristics of the reactor, have developed models using the process simulator Aspen Plus [101]. Aspen Plus is a problem-oriented input program that is used to facilitate the calculation of physical, chemical and biological processes. It can be used to describe processes involving solids in addition to vapour and liquid streams. Aspen Plus makes model creation and updating easier, since small sections of

complex and integrated systems can be created and tested as separate modules before they are integrated. This process simulator is equipped with a large property data bank containing the various stream properties required to model the material streams in a gasification plant, with an allowance for the addition of in-house property data. Where more sophisticated block abilities are required, they can be developed as FORTRAN subroutines.

Aspen Plus has been used to simulate coal conversion; examples include methanol synthesis [78,79], indirect coal liquefaction processes [80], integrated coal gasification combined cycle (IGCC) power plants [81], atmospheric fluidised-bed combustor processes [82], compartment fluidised-bed coal gasifiers [83], coal hydrogasification processes [84] and coal gasification simulation [85]. It has also been used to model and simulate a tyre pyrolysis unit within a gasification-based plant (Gómez et al. [103]).

However, the work that has been done on biomass gasification is less extensive. Mansaray et al. [86–88] used Aspen Plus to simulate a dual-distributor-type fluidised-bed rice husk gasifier. Two thermodynamic models were developed: a one-compartment model, where the hydrodynamic complexity of the fluidised-bed gasifier was neglected and an overall equilibrium approach was used; and a two-compartment model, where the complex hydrodynamic conditions presented within the gasification chamber were taken into account. The models were capable of predicting the reactor temperature, gas composition, gas higher heating value, and overall carbon conversion under various operating conditions, including bed height, fluidisation velocity, equivalence ratio, oxygen concentration in the fluidising gas, and rice husk moisture content. Because of the large amount of volatile material in biomass and the complexity of biomass reaction rate kinetics in fluidised-beds, the authors ignored char gasification and simulated the gasification process by assuming that biomass gasification follows the Gibbs equilibrium. The reactions considered in the development of the model were pyrolysis, partial combustion and gasification. Predictions of the core, annulus and exit temperatures, as well as the mole fractions of the combustible gas components and product-gas higher heating value, agreed reasonably well with experimental data. Correlations of the overall carbon conversion were not very good. The discrepancies between experimental and predicted overall carbon conversions were attributed to uncertainties in the sampling procedure.

Mathieu and Dubuisson [68] modelled wood gasification in a fluidised bed using Aspen Plus. The model was based on the minimisation of the Gibbs free energy and the process was uncoupled in pyrolysis, combustion, Boudouard reaction and gasification. The authors performed a sensitivity analysis and concluded that there is a critical air temperature above which preheating is no longer efficient, that there is an optimum oxygen factor, that the oxygen enrichment of air plays an efficient role under a certain value, and that the operating pressure has only a slight positive effect on process efficiency.

Mitta et al. [89] modelled a fluidised-bed tyre gasification plant with air and steam using Aspen Plus and validated their results with the gasification pilot plant located at the Chemical Engineering Department of the Technical University of Catalonia (UPC). Their gasification model was divided into three different stages: drying, devolatilisation-pyrolysis and gasification-combustion. Fig. 6 shows the Aspen Plus flowsheet of the model. When the raw material is fed, the first step is the heating and drying of the particles. A "RSTOIC" module was used to model this instantaneous drying. Due to the high content of volatiles in the tyre, the authors considered the devolatilisation step of its conversion. This devolatilisation process, namely the fast pyrolysis mechanism, produces volatile gases, tars and char. The "RYIELD" block was used to model the pyrolysis/devolatilisation part of the model. It was assumed that the total yield of volatiles equals the volatile content of the parent fuel determined by the proximate analysis. The "RGIBBS" reactor module was used to model the gasification and combustion reaction. The stream from the "RYIELD" block and the preheated oxygen and steam were directed into the "RGIBBS" module, which can predict the equilibrium composition of the produced gas from "RYIELD" at a specified temperature and pressure. The ash from the gasification process was removed from the "RGIBBS" module. In the model, an overall equilibrium approach was employed by neglecting the hydrodynamic complexity of the gasifier. Although higher hydrocarbons, tars and oils were produced in the gasifier, they were considered non-equilibrium products in order to decrease the complexity of the model. Therefore, CH_4 was the only hydrocarbon taken into consideration in the calculation. All of the results of the model were normalised to make them free from tars. The sulphur in the tyre was assumed to be converted mainly into H_2S. Steady-state conditions were assumed. The model was able to predict the composition of the produced gas under various working conditions, including the flow rate, composition and temperature of the feed materials, as well as the operating pressure and temperature.

Nikoo and Mahinpey [90] developed a model capable of predicting the steady-state performance of an atmospheric fluidised-bed gasifier by considering the hydrodynamic and reaction kinetics simultaneously. They used four Aspen Plus

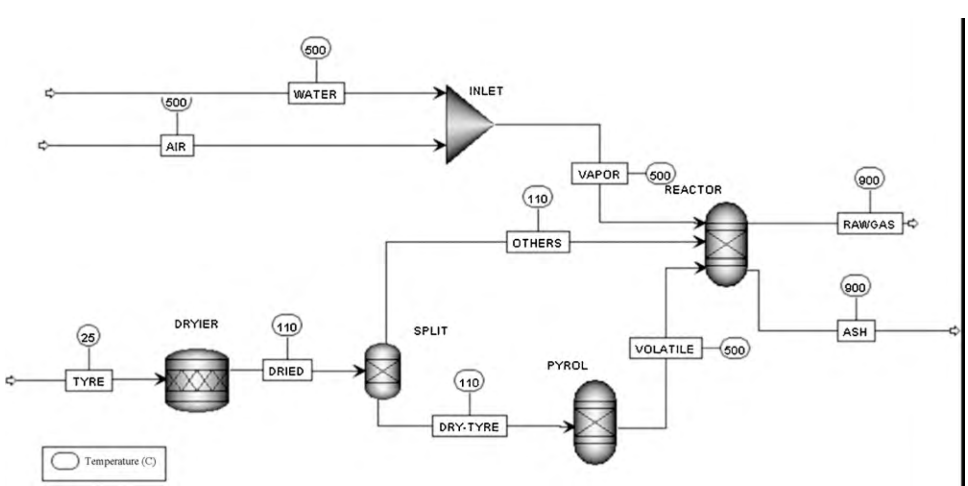


Fig. 6. Simulation diagram in Aspen Plus for a fluidised-bed tyre gasification process [89].

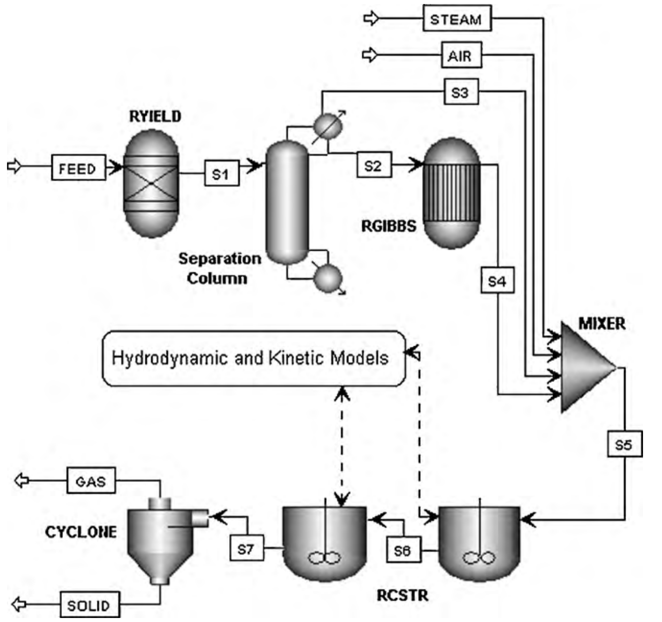


Fig. 7. Simulation diagram in Aspen Plus for an atmospheric fluidised-bed gasification [90].

reactor models and external FORTRAN subroutines for hydrodynamics and kinetics nested to simulate the gasification process (Fig. 7). The Aspen Plus yield reactor, "RYIELD", was used to simulate the decomposition of the feed. In this step, biomass was converted into its constituting components, including carbon, hydrogen, oxygen, sulphur, nitrogen and ash, by specifying the yield distribution according to the biomass ultimate analysis. A separation column model was used to separate the volatile materials and solids in order to perform the volatile reactions. The Aspen Plus Gibbs reactor, "RGIBBS", was used for volatile combustion, in conformity with the assumption that volatile reactions follow the Gibbs equilibrium. The Aspen Plus CSTR reactor, "RCSTR", performed char gasification using reaction kinetics, written as an external FORTRAN code. The hydrodynamic parameters divided the reactor into two regions, bed and freeboard, and each region was simulated by one "RCSTR". The authors validated their model using different sets of operating conditions for a lab-scale pine gasifier with air and steam. They found good qualitative agreement between the model's prediction and the experimental data, but they considered further improvements to the model, such as implementing tar production by defining non-equilibrium products in the "RGIBBS" reactor, as well as parameters considering mass transfer inside solid particles and heat transfer inside the particles, between phases, and between the material and the wall. However, the authors observed that the production of hydrogen increases with temperature, thereby enhancing carbon conversion efficiency. The equivalence ratio is directly proportional to CO_2 production and carbon conversion efficiency. Increasing the steam-to-biomass ratio increases hydrogen and carbon monoxide production and decreases CO_2 and carbon conversion efficiency. The average particle size, ranging from 0.25 to 0.75 mm, does not seem to contribute significantly to the composition of the product gases.

Other authors have worked with Aspen Plus to model the gasification process for coal and biomass. Yan and Rudolph [83] developed a model for a compartmented fluidised-bed coal gasifier process, Sudiro et al. [91] modelled the gasification process to obtain synthetic natural gas from petcoke. Paviet et al. [92] describe a very simple two-step model of chemical equilibrium in the wood biomass gasification process. Robinson and Luyben [93] presented an approximate gasifier model that can be used for dynamic analysis using Aspen Dynamics. They used a high-molecular-weight hydrocarbon that is present in the Aspen library as a pseudofuel and the proposed approximate model captured the essential macroscale thermal, flow, composition and pressure dynamics. Doherty et al. [94,95] developed a model for a circulating fluidised bed and studied the effect of varying the equivalence ratio, temperature, level of air preheating, biomass moisture and steam injection on the product gas composition, the gas heating value and the cold gas efficiency. Van der Meijden et al. [96] also used Aspen Plus as a modelling tool to quantify the differences in overall process efficiency for producing synthetic natural gas in three different gasifiers (entrained-flow, allothermal and circulating fluidised-bed gasifier).

4.4. Neural network gasification models

Non-mechanistic, non-equilibrium modelling using neural networks for biomass gasification has also been reported [97,98]. Artificial neural networks (ANN) have been extensively used in the fields of pattern recognition, signal processing, function approximation and process simulation. Sometimes a hybrid neural network (HNN) model is synthesised for process modelling [99]. This modelling approach usually combines a partial first-principles model, which describes certain characteristics of the process being simulated and involves a multilayer feedforward neural network (MFNN) that serves as an estimator of unmeasured process parameters that are difficult to model from first principles. MFNN is a universal function approximator, which has the ability to approximate any continuous function to an arbitrary precision even without a priori knowledge of the structure of the function to be approximated [100]. In Guo et al. [97], a HNN model was developed to simulate biomass gasification in a steam fluidised-bed gasifier. A series of gasification runs were conducted on a bench-scale facility, with four types of biomass as feedstock. The data obtained from these experiments were used to train the HNN model.

Brown et al. [98] developed an equilibrium reaction modelling approach for the efficient design of biomass gasifiers. Fuels and chars were defined as pseudospecies with properties derived from their ultimate analyses; tars were defined as a subset of known molecular species and their distribution was determined by equilibrium calculations. Non-equilibrium behaviour for gas, tar, and char formation was explained by reaction temperature differences for a complete set of stoichiometric equations. A nonlinear regression, with an artificial neural network, related changes in temperature differences to fuel composition and operational variables. This first-principles approach, illustrated with fluidised-bed reactor data, improves the accuracy of equilibrium calculations and reduces the amount of data required by preventing the NN from learning atomic and heat balances.

5. Conclusions

Models of several different types have been developed for gasification systems—kinetic, equilibrium and artificial neural networks. Unlike kinetic models that predict the progress and product composition at different positions along a reactor, an equilibrium model predicts the maximum achievable yield of a desired product from a reacting system. It also provides a useful design aid in evaluating the possible limiting behaviour of a complex reacting system that is difficult or unsafe to reproduce experimentally or in commercial operation. Equilibrium models are less computationally intensive than kinetic models and they are a useful tool for preliminary comparison. However, they cannot give highly accurate results for all cases.

Some authors, trying to avoid complex processes and aiming to develop the simplest possible model that incorporates the principal gasification reactions and the gross physical characteristics of the reactor, have developed models using the process simulator Aspen Plus.

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